

Enthalpy and entropy of activation and the heat effect of the ene reaction between 4-phenyl-1,2,4-triazoline-3,5-dione and 2,3-dimethyl-2-butene in solution

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Abstract

The rate of the fastest ene reaction between 4-phenyl-1,2,4-triazoline-3,5-dione (1) and 2,3-dimethyl-2-butene (2) is studied by means of stopped flow in solutions of benzene ($k_2 = 55.6 \pm 0.5$ and 90.5 ± 1.3 L mol⁻¹ s⁻¹ at 23.3 and 40°C) and 1,2-dichloroethane (335 ± 9 L mol⁻¹ s⁻¹ at 23.5°C). The enthalpy of reaction (-139.2 ± 0.6 kJ/mol in toluene and -150.2 ± 1.4 kJ/mol in 1,2-dichloroethane) and the enthalpy (20.0 ± 0.5 kJ/mol) and entropy (144 ± 2 J mol⁻¹ K⁻¹) of activation are determined. A clear correlation is observed between the reaction rate and ionization potential in a series of ene reactions of 4-phenyl-1,2,4-triazoline-3,5-dione with acyclic alkenes. © 2014 Pleiades Publishing, Ltd.

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Keywords

2,3-dimethyl-2-butene, 4-phenyl-1,2,4-triazoline-3,5-dione, ene synthesis, kinetics, thermochemistry